

An ecosystem modelling approach for deriving water quality criteria

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Abstract Ecological effects of chemicals on ecosystems are the result of direct effects of the chemical, determined in single-species toxicity testing, and indirect effects due to ecological interactions between species. Current experimental methods to account for such interactions are expensive. Hence, mathematical models of ecosystems have been proposed as an alternative. The use of these models often requires extensive calibration, which hampers their use as a general tool in ecological effect assessments. Here we present a novel ecosystem modelling approach which assesses effects of chemicals on ecosystems by integrating single-species toxicity test results and ecological interactions, without the need for calibration on case-specific data. The methodology is validated by comparing predicted ecological effects of copper in a freshwater planktonic ecosystem with an experimental ecosystem data set. Two main effects reflected by this data set (a decrease of cladocerans and an increase of small phytoplankton) which were unpredictable from single-species toxicity test results alone, were predicted accurately by the developed model. Effects on populations which don't interact directly with other populations, were predicted equally well by single-species toxicity test results as by the ecosystem model. The small amount of required data and the high predictive capacity can make this ecosystem modelling approach an efficient tool in water quality criteria derivation for chemicals.

Keywords Calibration; copper; ecological effect assessments; ecological interactions

Introduction

The development of water quality criteria for chemicals should entail the assessment of potential ecological effects at the ecosystem level. Ecological effects are determined by (1) the direct effects of the chemical on single species; and (2) ecological interactions between species (e.g., Chapman *et al.*, 2003). Relatively straightforward single-species tests are used to determine the former, while experimental ecosystems have been used to account for the latter. However, experimental ecosystems are very demanding in terms of required resources. Therefore, most ecological effect assessments of chemicals have been based exclusively on single-species toxicity test results, i.e. without accounting for ecological interactions between species. In those cases, single-species toxicity test results are extrapolated using statistical models or pragmatic assessment factors to estimate a safe environmental concentration (TGD, EU, 2003). Water quality criteria resulting from such effect assessments may be inaccurate (Forbes and Calow, 2002) because of the great importance of ecological interactions in determining ecological effects (Fleeger *et al.*, 2003).

For this reason, ecosystem models have been proposed to assess ecological effects (e.g., Traas *et al.*, 1998). However, these models are mostly calibrated on time-series data of one specific ecosystem (e.g., Bartell *et al.*, 1999), hence limiting their

applicability in other ecosystems. Parameters from ecosystem models are difficult to estimate (Loehle, 1997). From a mathematical point of view this is logical, since an ecosystem model consists of coupled equations with numerous feedback processes. One way to resolve this problem of limited parameter identifiability is to change the way in which ecosystem models are calibrated, i.e. by not relying on specific time-series data. Moreover, effect assessors are interested in ecological effects, and not in ecosystem dynamics. Unfortunately, predictions of such effects are never quantitatively validated.

In this paper, we present a novel ecosystem modelling approach to assess effects of chemicals on ecosystems based on (1) direct effects and (2) ecological interactions. The latter are represented by the ecosystem model equations in which single-species toxicity test results are incorporated to account for the former. The presented approach does not require calibration on specific time-series data. Instead, the model is parameterized using default values to qualitatively describe a number of very generic ecological concepts. This paper consists of two parts. First, the modelling approach is presented emphasizing underlying concepts and innovations, rather than equations. Second, the methodology is validated by comparing predicted ecological effects of copper in a freshwater planktonic ecosystem with a unique experimental ecosystem data set (Schaeffers, 2001).

Material and methods

General concept of the ecosystem model

A mechanistic dynamic ecosystem model was constructed in an object oriented framework. The model consists of a set of objects, where each object describes the growth of a population in terms of its total biomass using differential equations. By connecting different objects and defining the trophic links between them, a customized food web can be designed. The number of populations that can be modelled is unlimited and available objects are: phytoplankton, macrophytes, and zooplankton. Additionally, the growth kinetics of these objects are differentiated by parameter tuning (slow growing populations vs. fast growing populations). The phytoplankton object contains the processes photosynthesis, respiration, excretion, mortality, sinking, and grazing by zooplankton. The zooplankton object describes grazing on phytoplankton and detritus, defecation, respiration, excretion, and mortality. Based on the law of mass conservation, verification of model structure is done by a mass balance approach. All equations are based on Park (1974) and USEPA (2002). A brief overview of the main equations, parameters, and variables is provided in Table 1.

Population dynamics in the control

First, the model is used to simulate the population dynamics under control conditions, i.e. without toxicant addition. In contrast with other ecosystem modelling approaches (e.g. Traas *et al.*, 2004), no actual time series data is used to calibrate this ecosystem model. Instead, the model is parameterized so that it simulates a realistic succession of seasonal events. A synthesis of realistic planktonic events reported by different researchers working on a plethora of lakes is described in Sommer *et al.*, (1986). These events are, (1) spring bloom of small phytoplankton, (2) bloom of small zooplankton, resulting in a 'clear water phase', (3) a summer bloom of large phytoplankton, followed by (4) a bloom of larger zooplankton. To obtain this series of events, species are lumped into hypothetical populations based on their growth kinetics. The ecological interactions within the ecosystem studied are also defined following Sommer *et al.*, (1986): large-bodied zooplankton graze on both small and large

Table 1 Overview of the main equations of the constructed ecosystem model. For macrophytes, the phytoplankton equation is used, without the terms 'consumption by zooplankton' and 'sinking', and with different parameter values

$$\begin{aligned} \frac{dBio_{phyto}}{dt} &= \text{photosynthesis} - \text{respiration} - \text{excretion} - \text{mortality} - \text{consumption by zooplankton} - \text{sinking} \\ &= (PS_{max} - PS_{Limit} - Resp_0 \exp(\text{tempResp} \cdot \text{Temperature}) \\ &\quad - \text{exc}((1 - Lt_{Limit}) \cdot PS_{max} - PS_{Limit})) \cdot Bio_{phyto} \\ &\quad - ((\text{mort} + \text{ExcessT} + \text{Stress}) - \text{sed} - \text{SedAccel}) \cdot Bio_{phyto} - \sum \text{consumption}_j \end{aligned}$$

$$\begin{aligned} \frac{dBio_{zoo}}{dt} &= \text{consumption} - \text{defecation} - \text{respiration} - \text{excretion} - \text{mortality} \\ &= \sum \text{consumption}_i - \sum \text{defecation}_i - \text{consumption}_i - Resp_0 \cdot \text{tempLimit} \cdot Bio_{zoo} \\ &\quad - \text{resp}(\sum \text{consumption}_i - \sum \text{defecation}_i - \text{consumption}_i) - \text{excr} \cdot Resp_0 \cdot \text{tempLimit} \cdot Bio_{zoo} \\ &\quad - (\text{mort} + \exp(\frac{\text{Temperature} - T_{max}}{2})) \cdot Bio_{zoo} \end{aligned}$$

Parameter or Variable	Unit	Description
Bio _{phyto} and Bio _{zoo}	mg L ⁻¹	biomass concentration of phytoplankton and zooplankton, respectively
consumption _i and consumption _j	mg L ⁻¹ d ⁻¹	consumption of phytoplankton i and consumption by zooplankton j
defecation _i	-	fraction egested of food source
exc and excr	-	excretion/photosynthesis ratio and excretion/respiration ratio
ExcessT	d ⁻¹	increased mortality due to suboptimal temperature
LtLimit	-	light limitation of phytoplankton growth
mort	d ⁻¹	intrinsic mortality rate for given population
PSLimit	-	limitation of phytoplankton photosynthesis due to suboptimal nutrients, light, temperature, pH, and oxygen
PSmax	d ⁻¹	maximum photosynthetic rate of given phytoplankton
resp	-	fraction of energy lost to dynamic action
Resp0	d ⁻¹	intrinsic respiration rate
sed	d ⁻¹	intrinsic sinking rate of phytoplankton
SedAccel	-	increased sinking due to physiological stress
Stress	d ⁻¹	increased mortality due to physiological stress
tempLimit	-	temperature correction for zooplankton respiration and temperature limitation of considered process (e.g. photosynthesis)
tempResp	-	exponential temperature coefficient of phytoplankton respiration
Temperature	°C	water temperature
Tmax	°C	maximum tolerated temperature of considered zooplankton

phytoplankton, while small-bodied zooplankton can only ingest small phytoplankton. Given these ecological constraints, default parameter values provided by USEPA (2002) were changed within a 10% range until this succession of seasonal events was predicted. Note that this is a qualitative calibration procedure solely relying on the model equations and generic ecological concepts.

Population dynamics in different toxicant treatments

The population dynamics at a given toxicant concentration were predicted by changing growth rate-determining parameters of the populations in the ecosystem model, using concentration-response functions. These parameters are the mortality rate (for zooplankton and macrophytes) and the photosynthesis rate (for phytoplankton and macrophytes). Single-species toxicity test results on zooplankton mortality and phytoplankton and

macrophyte growth rate are parameters used in these concentration-response functions:

$$PS \max_c = \frac{PS \max}{1 + \left(\frac{c}{EC_{50,PS \max}} \right)^{\text{slope}}} \quad (1)$$

$$\text{mort} = \frac{1}{\text{time}} \cdot \ln \left\{ 1 + \left(\frac{c}{LC_{50}} \right)^{\text{slope}} \right\} \quad (2)$$

with: $PS \max$ = maximum photosynthetic rate of phytoplankton in control conditions; $PS \max_c$ = maximum photosynthetic rate of phytoplankton at a toxicant concentration c ; $EC_{50,PS \max}$ = concentration at which 50% effect on PS_{\max} is observed in a single-species toxicity test; LC_{50} = concentration at which 50% mortality is observed in a single-species toxicity test; slope = slope of the considered concentration-response data obtained in a single-species toxicity test; time = duration of the single-species toxicity test in which the LC_{50} was determined; and mort = mortality rate of given zooplankton.

As such, direct effects of a toxicant, as reflected by single-species toxicity test results, are incorporated in the ecosystem model equations. The choice for logistic functions originates from the sigmoid pattern that single-species toxicity test results exhibit for most toxicants (Newman and Unger, 2003). Variability on single-species toxicity test results is propagated in the simulation results with a Monte Carlo approach (Cullen and Frey, 1999). As such, population dynamics at a concentration c are simulated n times, with “ n ” the number of shots.

Modelling ecological effects

Ecological effects are quantified by comparing population dynamics of the exposed system with population dynamics at control. For each population, the average biomass is calculated at the control, as well as at the different toxicant concentrations, and this over the whole simulation period. This allows to calculate relative differences (RDs) of the average biomass of the populations at each toxicant concentration c :

$$RD_{\text{population}} = \frac{X_{\text{population},c} X_{\text{population,control}}}{X_{\text{population,control}}} \quad (3)$$

with $X_{\text{population},c}$ the average biomass in time of green algae at concentration c (mg L^{-1}), and $X_{\text{population,control}}$ the average biomass in time of green algae at control (mg L^{-1}).

As such, RDs could be calculated for each population at each concentration c .

NOEC calculation

Because 20% is the minimum detectable difference for most population characteristics in the field (Suter II, 1993), RD -values of -0.2 or lower are considered as detectable decreases of biomass. Similarly, RD -values of 0.2 or higher are considered as detectable increases of biomass. Given the variability propagation discussed in the previous paragraph, n RDs are calculated per population and per toxicant concentration. The no observed effect concentration ($NOEC_{\alpha}$) for decrease of a populations' biomass is defined as the highest concentration at which less than $100 \cdot (1 - \alpha)$ % of the RD values for this population were ≤ -0.2 . This percentile is calculated by ranking the n RD values using the mean plotting position (Davison and Hinkley, 1997). The α -value can be considered equivalent to the significance level of classical statistical testing. Similarly, the $NOEC_{\alpha}$ for increase of a population, is defined as the largest concentration at which less than $100 \cdot (1 - \alpha)$ % of the RD values for this population were ≥ 0.2 . The ecosystem- $NOEC_{\alpha}$ is defined as the lowest $NOEC_{\alpha}$ of all populations. In this paper, a default alpha value of

0.35 was taken. The effect of the chosen α -value on predictions is examined elsewhere (De Laender *et al.*, submitted a, b).

Copper effects in aquatic microcosms

The developed methodology was used to predict population-NOECs for copper in a planktonic freshwater ecosystem (Figure 1A), for which a unique experimental ecosystem data set is available (Schaeffers, 2001). Indoor aquatic microcosms with a volume of about 1 m³, were permanently exposed to six levels of copper sulphate (5, 10, 20, 40, 80 and 160 $\mu\text{g Cu L}^{-1}$) while measuring biomass dynamics of various species. The biomass concentration data were lumped into two slow growing zooplankton populations (cladocerans and copepods), fast growing zooplankton (rotifers), spring phytoplankton, summer phytoplankton, and one macrophyte. From this data set, RDs and NOECs were calculated using the same methodology as that used for the model predictions. In the remainder of

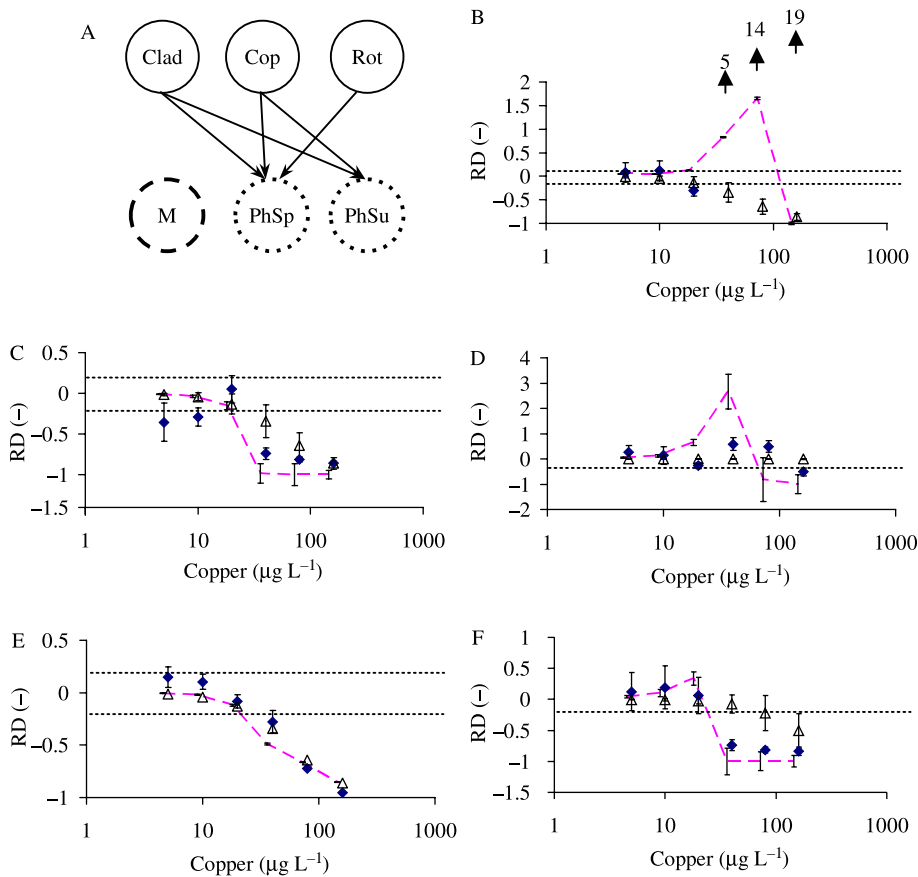


Figure 1 A: Food web of the considered ecosystem in which only feeding interactions are presented, i.e. grazing; 'Rot' stands for small zooplankton, rotifers. 1B–F: Biomass changes, relative to control (RD), as a function of copper concentration for the populations in the ecosystem: spring phytoplankton, PhSp (B); summer phytoplankton, PhSu (C); large zooplankton1, copepods, Cop (D); large zooplankton2, cladocerans, Clad (F); the macrophyte, M (E). Observations from a microcosm experiment and associated standard errors are indicated by \blacklozenge and error bars, respectively. Dashed lines give predicted values. Dotted lines indicate $\text{RD} = -0.2$ and/or $+0.2$. The arrows in (B) point to observed RD values that are larger than 2. Direct effects, as given by single-species toxicity test results are indicated by Δ

this paper, these are termed ‘observed’ *RDs* and *NOECs*, because they are derived from the microcosm observations.

Values of *RD* and *NOEC* for the six populations in the considered ecosystem were predicted with the ecosystem model and compared to the observed *RDs* and *NOECs*. Single-species toxicity test results describing the effects of copper on aquatic biota were collected from literature. Because of the known influence of water characteristics (e.g., pH, water hardness and dissolved organic carbon (DOC) on copper toxicity (e.g., Erickson *et al.*, 1996; De Schamphelaere and Janssen, 2002), all used single-species toxicity test results were normalized to the water characteristics of the microcosm study as in De Laender *et al.*, (submitted a). In the absence of adequate single-species toxicity test results, effects on the macrophyte mortality rate were taken from a previous study examining copper effects on the same macrophyte (De Laender *et al.*, submitted c). A slope value for concentration-response curves of metals was taken from Smit *et al.* (2001). A 10% coefficient of variation on all single-species toxicity test results were propagated by Monte-Carlo simulation.

Results and discussion

RD predictions

In general, observed and predicted *RD* values are in fair agreement (Figure 1B–F). The uncertainty on these predictions, as given by the corresponding error bars, is comparable with the uncertainty on single-species toxicity test results (Figure 1B–F). The rule of convergence (Melching, 1995) showed that variance on the model output stabilized after 60–80 shots. The drastic biomass decreases of cladocerans and phytoplankton_{summer} at copper concentrations $> 20 \mu\text{g L}^{-1}$ are accurately predicted by the model. To illustrate the necessity of including ecological interactions to predict ecological effects in this system, the direct effect of copper, as predicted by single-species toxicity test results alone, is also plotted (Figure 1B–F: triangular symbols). Clearly, at concentrations of 40 and $80 \mu\text{g L}^{-1}$, direct effects alone cannot explain the observed biomass decrease of cladocerans and phytoplankton_{summer}.

The predicted increase of phytoplankton_{spring} biomass at copper concentrations of 40 and $80 \mu\text{g L}^{-1}$ is confirmed by the microcosm data, although the observed increase (up to 1000%) is much higher than the predicted increase (100 to 200%). Nevertheless, both predicted and observed increases are $>20\%$ and as such indicate an observable effect. The direct effect alone erroneously indicates a decrease of phytoplankton_{spring} biomass. Apparently, the ecological interactions within this system result in an ecological effect which is opposite to the direct effect: the reduction of cladoceran biomass lowers the grazing pressure on phytoplankton in general. Thus benefits the phytoplankton_{spring}. The same mechanism has also been observed by other authors in experimental ecosystems exposed to metal mixtures (Jak *et al.*, 1996) and pesticides (Hanazato, 2001). The reason why phytoplankton_{summer} does not benefit from this reduced grazing pressure, while phytoplankton_{spring} does, may result from the competitive advantage for nutrients of the latter at elevated nutrient levels (Sommer *et al.*, 1986). Indeed, the loss of (living) biomass resulting from exposure to copper, increases (dead) organic matter and nutrient concentrations.

At concentrations $\leq 10 \mu\text{g L}^{-1}$, *RDs* of copepods are predicted correctly. At $40 \mu\text{g L}^{-1}$, the ecosystem model predicts a large increase of copepods, while observations only indicate a small increase for this population at that concentration. Comparison of these ecosystem model predictions with the direct effects as predicted from single-species toxicity test results alone, indicates that the inclusion of ecological interactions did not improve the effect assessment for copepods. Yet, this inclusion did not impede the correct prediction of a biomass decrease at $160 \mu\text{g L}^{-1}$.

The biomass decrease of the macrophyte is slightly overestimated by the ecosystem model, especially at concentrations $\leq 80 \mu\text{g L}^{-1}$. Direct effects did not differ too much from these ecosystem model predictions, indicating that ecological interactions had a limited influence on ecological effects on this population. This is logical since the macrophyte has no feeding relationships with other populations (Figure 1A). The only ecological interaction in which the macrophyte takes part is the competition for nutrients with phytoplankton.

Predictions of rotifer *RDs* were different from observed *RDs* (results not shown). This poor prediction performance can be explained by the very low rotifer densities ($< 0.5 \mu\text{g L}^{-1}$) in the microcosm experiment (Schaeffers, 2001). Loss of a single organism thus has a serious impact on *RD* values. It is therefore questionable whether the *RD* values for rotifers, as derived from the microcosm data, give a reliable reflection of copper effects on this population. For the same reason, Schaeffers (2001) was not able either to calculate a reliable $\text{NOEC}_{\text{rotifers}}$. Hence, rotifer data and predictions were omitted for NOEC determination.

NOEC predictions

Because predicted *RDs* were found to be fairly accurate for most populations, NOEC predictions showed good correspondence with observed NOECs too. The only exception is the predicted $\text{NOEC}_{\text{macrophyte decrease}}$ of $20 \mu\text{g L}^{-1}$, which is lower than the observed one ($40 \mu\text{g L}^{-1}$). Possible reasons for this anomaly are (1) use of a phytoplankton toxicity data in the toxic effect sub-model for macrophytes, as discussed in the ‘material and methods’ section; (2) incorporation of both mortality and photosynthesis effects in the toxic effect sub-model for macrophytes. Previous work indicates that, for invertebrates, inclusion of effects on both mortality and sublethal endpoints results in overestimation of effects on invertebrates (De Laender *et al.*, submitted a). Inclusion of mortality effects alone did result in superior predictions. Hence, inclusion of mortality effects alone could have resulted in better NOEC -predictions for this macrophyte.

The slight underestimation of the $\text{NOEC}_{\text{macrophyte decrease}}$ is of little importance in the determination of the ecosystem- NOEC . The latter is defined as the lowest population- NOEC , and is thus determined by populations other than the macrophyte. Indeed, the correct prediction of the NOECs of the more sensitive populations results in an accurate ecosystem- NOEC of $20 \mu\text{g L}^{-1}$. As noted by Pastorok *et al.* (2003), the accuracy of this type of models is highest at the lowest exposure concentrations. As stated before, ecological effects are determined by (1) direct effects; and (2) ecological interactions. In a system with many different ecological interactions or many direct effects, prediction of ecological effects will be more difficult. The reason for this is the increasing stochasticity resulting from an increasing number of processes occurring simultaneously. The fact that at higher concentrations more populations experience direct effects, makes predictions of ecological effects at those concentrations more difficult.

In this work, population- NOECs were derived from the experimental microcosm data - termed ‘observed NOECs ’ - to allow comparison with predicted population- NOECs . Comparison of these ‘observed NOECs ’ with NOECs derived by Schaeffers (2001) using a different statistical technique shows a good agreement. Apparently, treating the microcosm data in two completely different ways results in the same NOEC , with the exception of the $\text{NOEC}_{\text{macrophyte decrease}}$. The fact that Schaeffers (2001) only used the macrophyte biomass concentration measured on the last day of the experiment for NOEC calculation, may have influenced the result for this population. The biomass of all the other populations was measured throughout the complete period of the experiment and subsequently used for NOEC calculation.

Conclusions

In this paper, we developed a novel approach to predict ecological effects of chemicals in aquatic ecosystems. The approach is based on an ecosystem model, generic ecological concepts, and single-species toxicity test results. As such, it can perform predictions, without the need for experimental ecosystem data, which are classically expensive to monitor. Ecosystem model predictions of ecological effects of copper in a freshwater ecosystem were remarkably accurate. For most populations, predictions of the difference of the average biomasses at different toxicant concentrations, relative to the control biomass (*RD*) were accurate, or at least indicated the same trend as the experimental microcosm data. The few inaccurate *RD*-predictions did not affect the accuracy of most population-NOEC predictions. These predictions were significantly better than predictions based on single-species toxicity test results alone. This again confirms the importance of accounting for ecological interactions when conducting ecological effect assessments.

It is concluded that single-species toxicity test results and very generic ecological concepts are sufficient to accurately predict ecological effects of copper in the system studied. Because of the ubiquity of single-species toxicity test results it is suggested that the approach presented here may contribute to an improved procedure to derive water quality criteria.

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